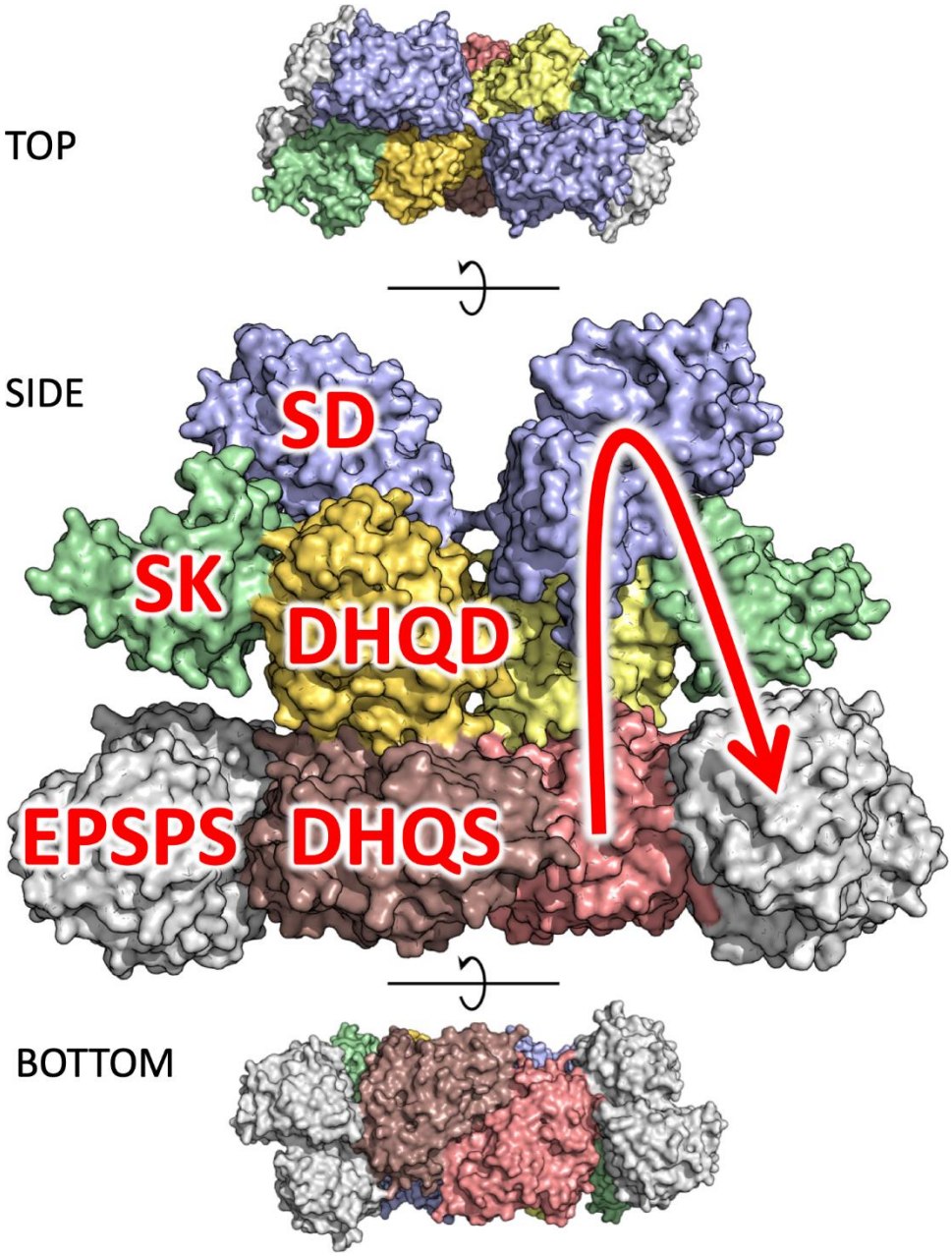
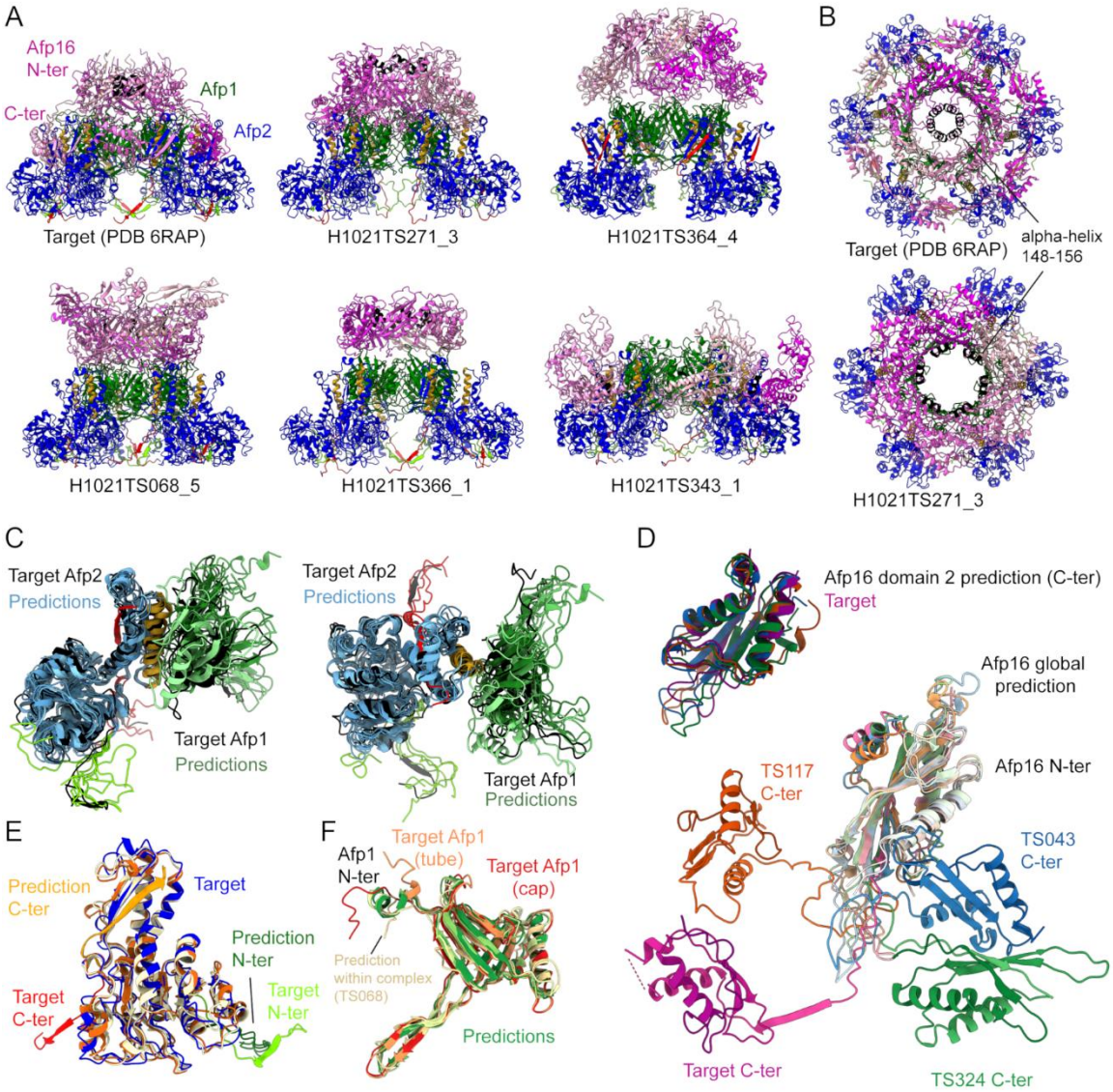
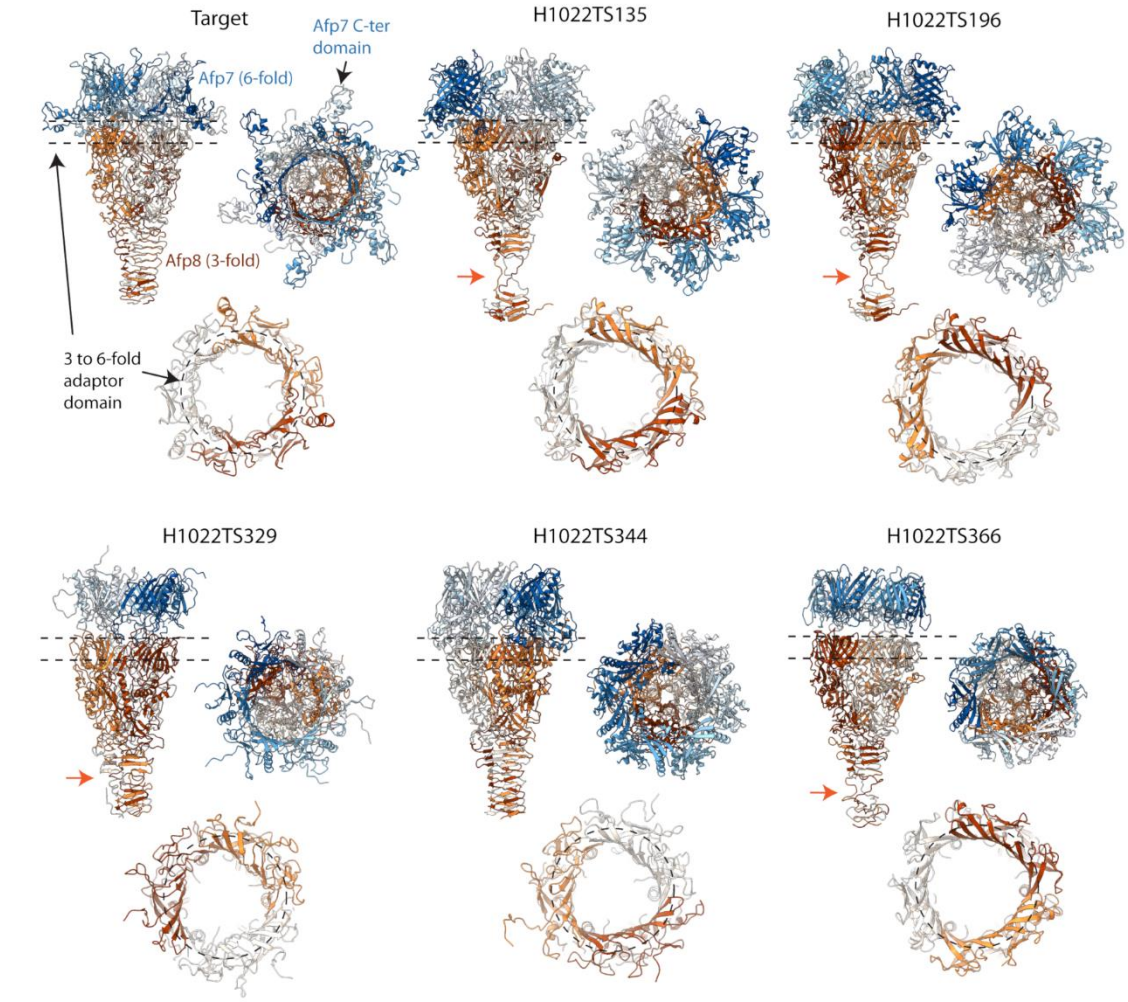
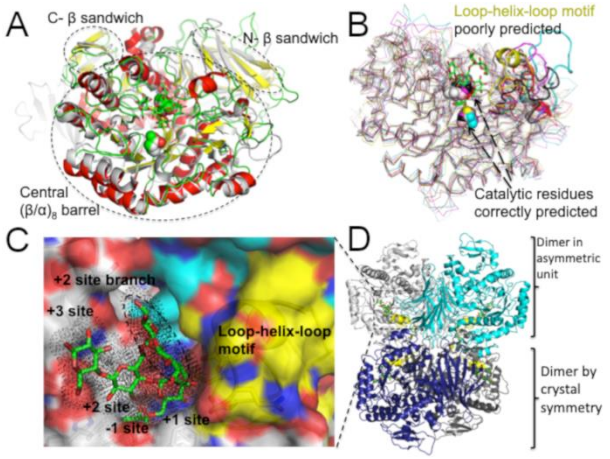
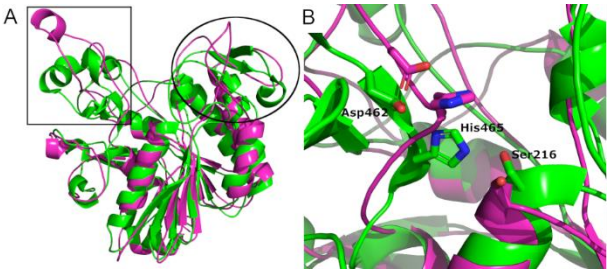
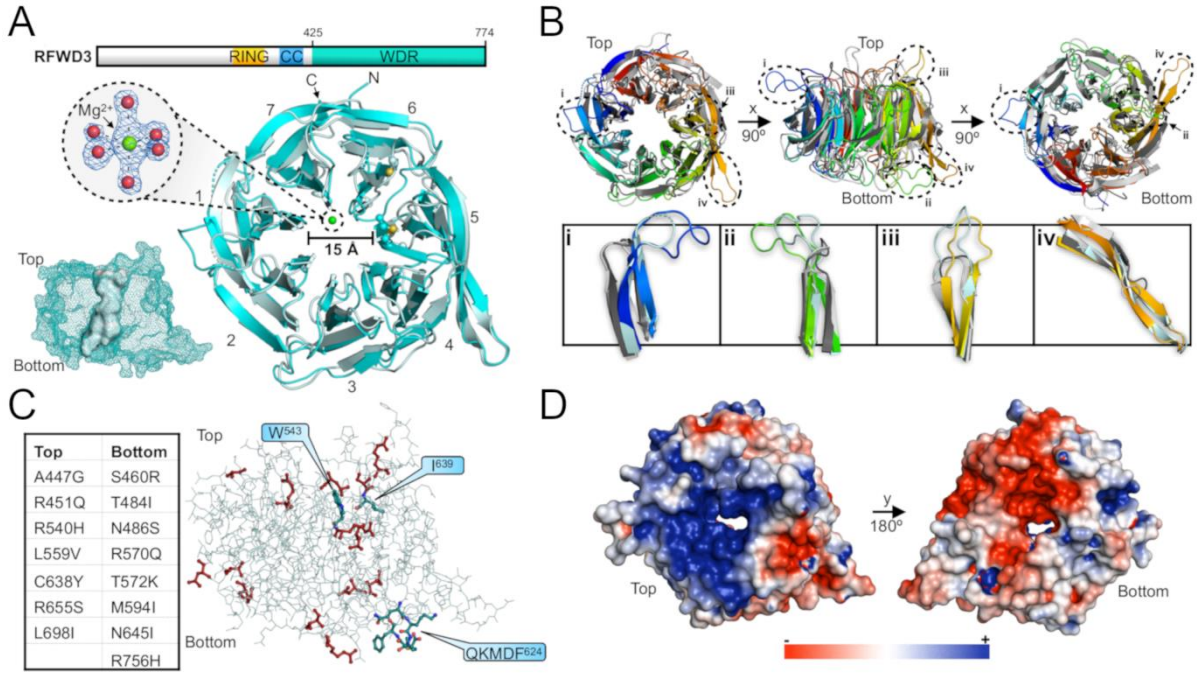

TOP
SIDE
SD
SK
DHQD
EPSPS
DHQS
BOTTOM


A
Afp16
N-ter
Afp1
C-ter
Afp2
Target (PDB 6RAP)
H1021TS271_3
H1021TS364_4
H1021TS068_5
H1021TS366_1
H1021TS343_1
B
Target (PDB 6RAP)
alpha-helix
148-156
H1021TS271_3
C
Target Afp2
Predictions
Target Afp1
Predictions
Target Afp2
Predictions
Target Afp1
Predictions
D
Afp16 domain 2 prediction (C-ter)
Target
Afp16 global
prediction
Afp16 N-ter
TS117
C-ter
TS043
C-ter
Target C-ter
TS324 C-ter
E
Prediction
C-ter
Target
Prediction
N-ter
Target
C-ter
Target
N-ter
F
Afp1
N-ter
Target Afp1
(tube)
Target Afp1
(cap)
Prediction
within complex
(TS068)
Predictions

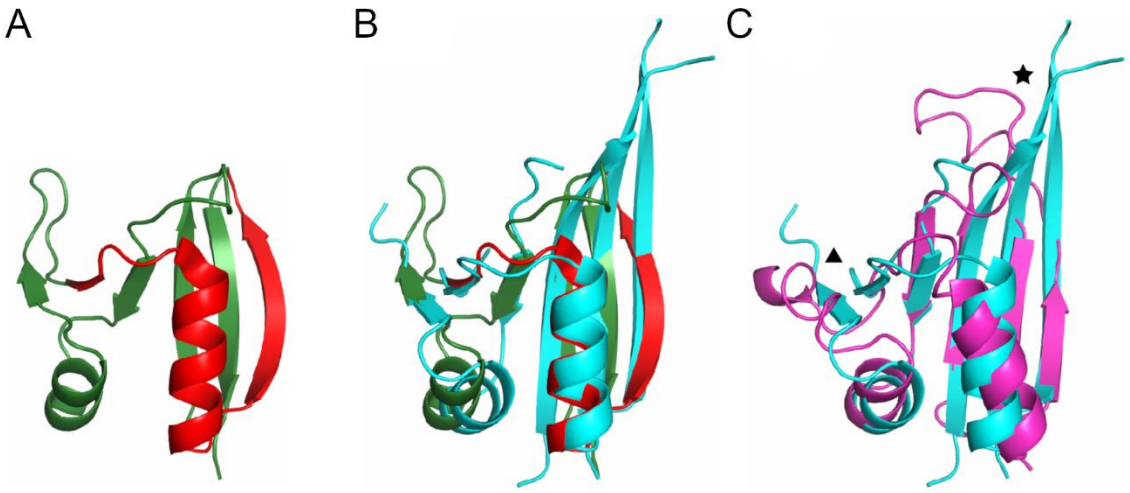

Target
Afp7 C-ter domain
Afp7 (6-fold)
Afp8 (3-fold)
3 to 6-fold adaptor domain
H1022TS135
H1022TS196
H1022TS329
H1022TS344
H1022TS366

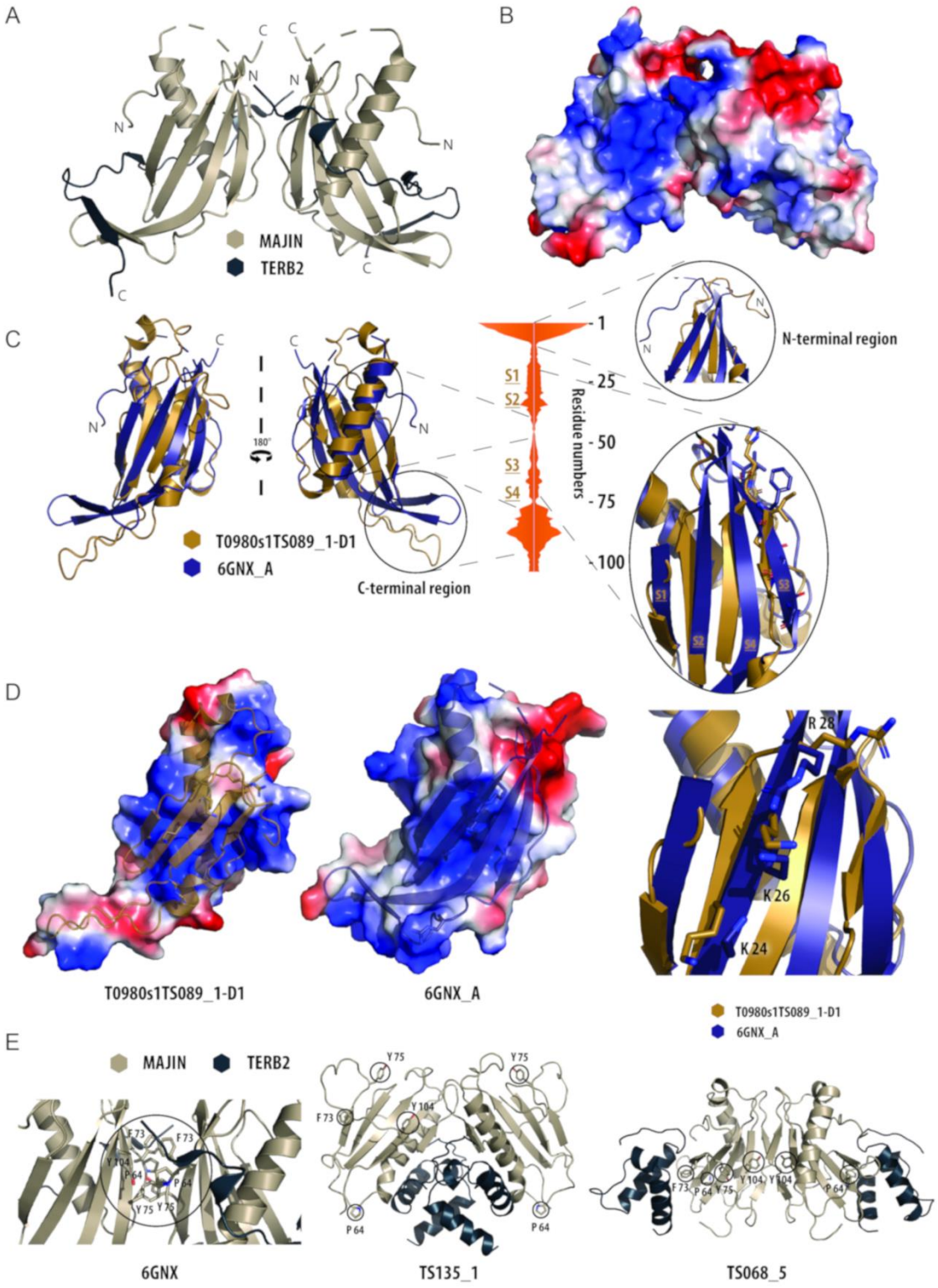

A
C- β sandwich
N- β sandwich
Central (β/α)8 barrel
B
Loop-helix-loop motif poorly predicted
Catalytic residues correctly predicted
C
+2 site branch
+3 site
Loop-helix-loop motif
+2 site
-1 site
+1 site
D
Dimer in asymmetric unit
Dimer by crystal symmetry

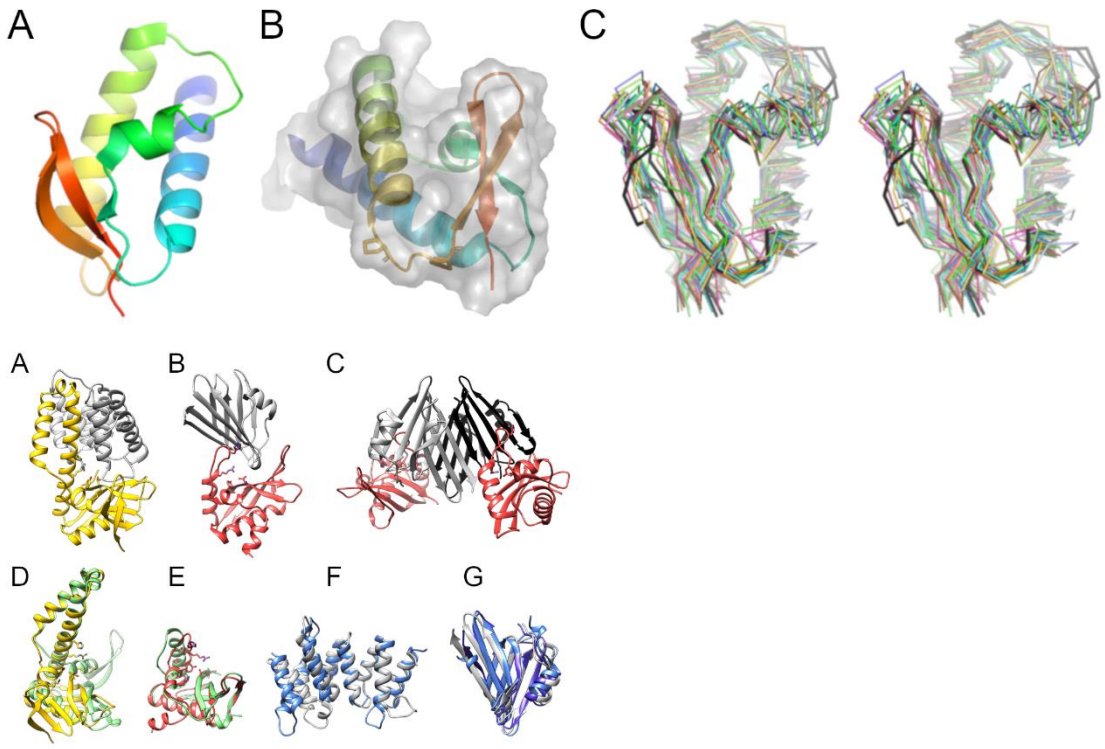

A
B
Asp462
His465
Ser216

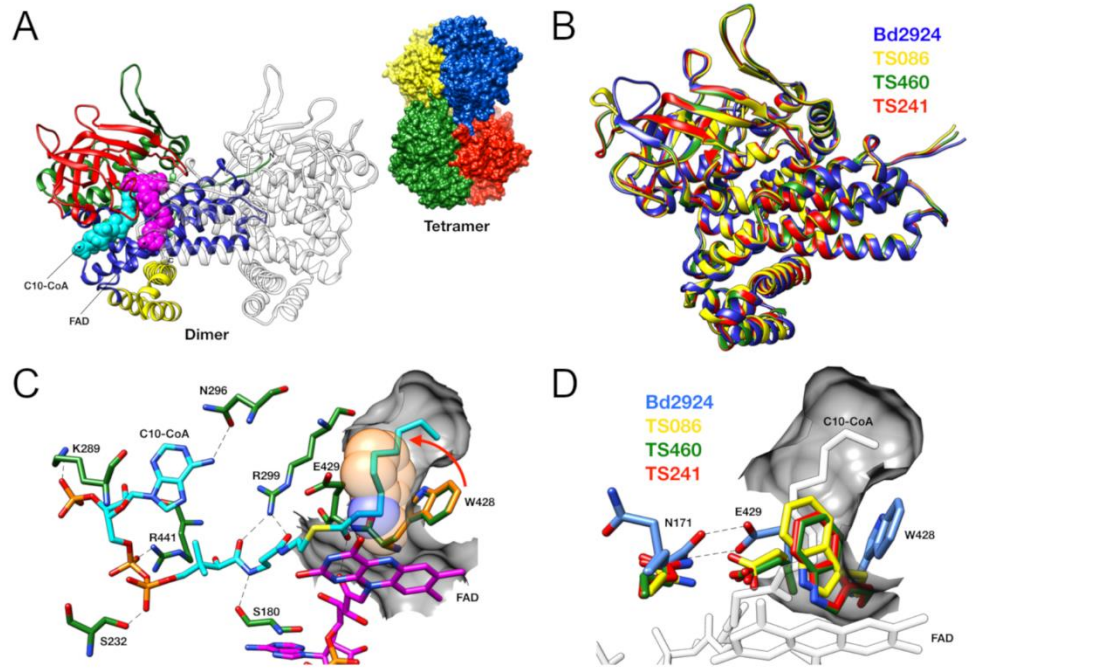


Top	Bottom
A447G	S460R
R451Q	T484I
R540H	N486S
L559V	R570Q
C638Y	T572K
R655S	M594I
L698I	N645I
	R756H




A
MAJIN
TERB2
B
C
180°
T0980s1TS089_1-D1
6GNX_A
C-terminal region
S1
S2
S3
S4
Residue numbers
1
25
50
75
100
N-terminal region
D
T0980s1TS089_1-D1
6GNX_A
R 28
K 26
K 24
T0980s1TS089_1-D1
6GNX_A
E
MAJIN
TERB2
F 73
Y 104
P 64
Y 75
6GNX
TS135_1
TS068_5


A
B
C
A
B
C
D
E
F
G


A
C10-CoA
FAD
Dimer
Tetramer
B
Bd2924
TS086
TS460
TS241
C
N296
C10-CoA
K289
R299
E429
W428
R441
FAD
S180
S232
D
Bd2924
TS086
TS460
TS241
C10-CoA
N171
E429
W428
FAD

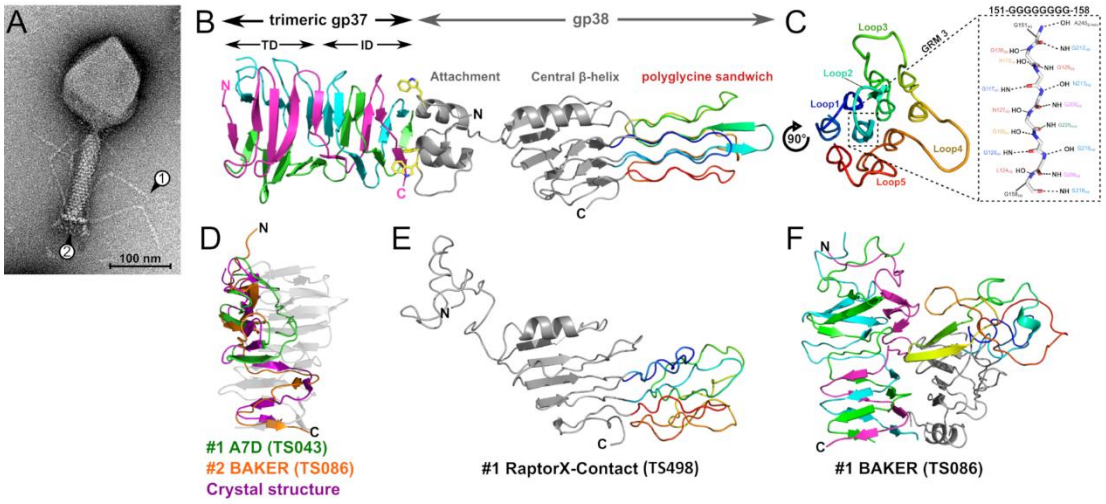

A
100 nm
B
trimeric gp37
gp38
TD
ID
Attachment
Central β-helix
polyglycine sandwich
C
Loop3
GPM 3
Loop2
Loop1
Loop4
Loop5
90°
151-GGGGGGGG-158
D
#1 A7D (TS043)
#2 BAKER (TS086)
Crystal structure
E
#1 RaptorX-Contact (TS498)
F
#1 BAKER (TS086)

Table 1. CASP13 target highlights. Columns indicate Target ID, PDB ID, Experimental Method, Resolution, Stoichiometry, Size and CASP13 assessment results. For each target, the accuracy of the best model 1 is provided both at the level of individual protomers (best GDT-TS and corresponding IDDT score) and full assembly (best QS-score).

Target	PDB	Method	Resolution (Å)	Stoichiometry	Size	CASP13 assessment		
						Protomer		Assembly
						GDT-TS	IDDT	QS-score
T0969	6CCI	X-ray	1.85	A1	487	58.19	0.51	-
T0958	6BTC	X-ray	2.18	A1	96	80.84	0.69	-
T0954	6CVZ	X-ray	1.80	A1	350	72.02	0.66	-
T0970	6G57	X-ray	2.80	A2	97	67.94	0.28	0.64
T0961	6SD8	X-ray	1.50	A4	505	91.65	0.80	0.91
T1009	6DRU	X-ray	2.70	A2	718	71.24	0.64	0.18
T0999	N/A	X-ray	3.00	A2	1589	80.39	0.73	0.82
H0953	6F45	X-ray	1.70	A3B1	72 249	54.48 40.12	0.63 0.40	0.37
H0957	6CP8	X-ray	2.20	A1B1	163 164	45.22 60.97	0.57 0.57	0.07
H0968	6CP9	X-ray	2.55	A2B2	126 116	71.40 78.70	0.61 0.66	0.14
H0980	6GNX	X-ray	2.90	A2B2	111 52	54.81 -	0.45 -	0.08
H1021	6RAP	EM	3.30	A6B6C6	149 354 295	75.67 68.70 36.77	0.65 0.58 0.57	0.33
H1022	6RBK	EM	3.40	A6B3	229 529	43.61 62.25	0.55 0.59	0.43

TABLE S1. CASP13 target providers.

#	Contibutor	Country	Institution	#	Contibutor	Country	Institution
1	Tom Peat	Australia	CSIRO	19	Xiaochen Bai	USA	UT SouthWest MC
2	Leila Lo Leggio	Denmark	U Kobenhavn	20	George Minasov	USA	NorthWestern U
3	Ambroise Desfosses	France	IBS, Grenoble	21	Lindsey Spiegelman	USA	UC San Diego
4	Marianne Ilbert	France	CNRS, Paris	22	Chi-Lin Tsai	USA	UTMD Anderson
5	Michael Groll	Germany	Tech U Munchen	23	Manal Swairjo	USA	San Diego State
6	Andrei Lupas, Marcus Hartmann	Germany	Max Planck Tübingen	24	Andrzej Joachimiak, Karolina Michalska, Kemin Tan	USA	Argonne Lab
7	Noa Keren	Israel	Ben Gurion U	25	Thomas Szyperski	USA	U Washington
8	Kaspars Tars	Latvia	BRCS, Riga	26	Gaetano Montelione	USA	U Rutgers
9	Shabir Najmudin	Portugal	U Lisbon	27	Garry Buchko	USA	Pacific NW Natl Lab
10	Stefan Arold	Saudi Arabia	KAUST	28	Petr Leiman	USA	U Texas MB
11	Mark van Raaij	Spain	CSIS, Madrid	29	Damian Ekiert	USA	New York U
12	Tilman Schirmer	Switzerland	U Basel	30	George Phillips, Jonathan Clinger, Mitchell Miller	USA	U Rice
13	Brian Trevor Sewell	So. Africa	U Cape Town	31	Hong Zhou	USA	UC Los Angeles
14	Brian Marsden	UK /Canada	SGC, Oxford/Toronto	32	Hongnan Cao	USA	Georgia I Tech
15	Owen Davies	UK	U Newcastle	33	Henrique Pereira	USA	L Berkeley Lab
16	Arnaud Basle	UK	U Newcastle	34	Oliver Clarke	USA	Columbia U
17	Andrew Lovering	UK	U Birmingham	35	Phoebe Rice	USA	U Chicago
18	Adam Frost	USA	UC San Francisco	36	Marcus Alahuhta	USA	Natl Renewable Energy Lab